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ABSTRACT

The WINERED spectrograph requires a large (9 cm x 9 cm aperture), 70º blaze ZnSe immersion grating to achieve a resolution of ~100,000. It will be implemented as a mosaic of 3 gratings of aperture 3 cm x 9 cm. LLNL is diamond machining a subscale prototype (2.3 cm x 5.0 cm aperture) to demonstrate feasibility. This is a 10x increase in the size of gratings machined at LLNL.

The first cutting of the grating had large wave front errors due to non-working thermal control. After repairs we recut a grating with an rms wavefront error of 0.11 wave @633 nm, which meets WINERED's full aperture requirement. The first cutting had good quality grooves, but the recut showed bad chipping. A second recut after polishing away the grating had pitted groove faces. It is known that diamond machining and mechanical polishing create subsurface damage. This damage can cause brittle fracture during subsequent machining. We plan to chemically etch ZnSe substrates to remove damaged layers prior to machining our next gratings.

Keywords: immersion grating, zinc selenide, diamond machining, WINERED, subsurface damage

1. INTRODUCTION

An immersion grating (a diffraction grating immersed in a high index material) is a valuable tool for increasing the resolution of an astronomical spectrograph. The concept was first discussed over 55 years ago[1] and, the first attempts at realization occurred over 15 years ago[2]. With recent advances in technology they are starting to appear in astronomical instruments[3,4,5]. Immersion increases dispersion and resolution proportional to the refractive index, so there is much benefit in utilizing high index materials. These are more numerous in the infrared region of the spectrum.

Most of the immersion gratings reported to date have been fabricated in silicon[6,7,8]. Silicon is unique in that chemical etching achieves high anisotropy, which leads to smooth, flat grooves whose orientation is determined by crystal axes. Efforts to fabricate silicon gratings also benefit from the high level of technology and the infrastructure developed for the worldwide semiconductor industry. There are situations where spectroscopy is required outside of the wavelengths where silicon has high transmission and other materials must be employed along with other fabrication techniques.

At LLNL a machining technique was developed to cut immersion gratings in germanium[9]. It has since been applied to zinc selenide and gallium phosphide[10].

The optical design[11] for WINERED, a high-resolution near infrared spectrograph under development in Japan, requires a large (90 mm x 90 mm entrance aperture) 70º blaze ZnSe immersion grating. This paper will report on efforts to machine a subscale prototype (23 mm x 50 mm entrance aperture) grating. Section 2 provides background and lists the performance requirements on the ZnSe grating. Sections 3, 4, and 5 each describe a separate effort at cutting the grating, the outcome of each effort, and the lessons learned. Section 6 presents conclusions and recommendations for machining a large, high quality ZnSe grating.

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2. BACKGROUND- AN IMMERSION GRATING FOR THE WINERED SPECTROGRAPH

The WINERED spectrograph[12] is designed to be an extremely high resolution instrument optimized for the short near infrared (NIR) region from 0.9 to 1.35 µm. The high dispersion of an immersion grating allows a resolution of ~100,000 to be attained in a compact, portable spectrograph. Because the transmission of silicon cuts off below 1.1 µm, it cannot be used for the grating substrate. Zinc selenide was chosen instead due to its high refractive index, good transmission, and its commercial availability in large sizes. ZnSe does not etch anisotropically, so other fabrication techniques must be used.

The baseline optical design for WINERED calls for a ZnSe grating blazed at 70º with a groove density of 31.52 lines per mm (groove period is 31.73 µm). The collimated beam is 70 mm in diameter at the grating. To allow for an angle of separation of a few degrees between input and output beams and also to allow for beam spread due to grating dispersion the clear aperture is 90 x 90 mm. This is a very large grating. Fabricating the grating in a single piece of ZnSe requires a thicker slab of material than is commercially available. Another difficulty is that absorption and scatter in the long optical path in ZnSe causes excess attenuation reducing the throughput and the spectral resolution. So the design incorporates a mosaic of three gratings with apertures of 30 x 90 mm.

A key specification of a grating is the allowable wavefront error in the diffracted beam. The total wavefront error produced by the refractive optics of WINERED is about 1.0 wave peak to valley (p-v) at 1.0 um. So the wavefront error contributed by the grating must be < 1.0 wave p-v over the entire 70mm diameter collimated beam.

There is another requirement on wavefront error, which applies over subapertures of the collimated beam. WINERED employs wide slits for minimizing throughput loss for seeing limited point sources. This means that the spectral resolution is determined by the silt width[13] not the diffraction limit. The equivalent diffraction limited beam size for R=100,000 is about 7.5mm for the WINERED grating. So the wavefront error within any 7.5mm circular aperture across the collimated beam must be < 0.25 wave p-v or equivalently (for random surface errors) <0.071 wave rms at 1.0 µm.

The first report of a ZnSe grating was by Rayner[14]. His grating was directly ruled with a diamond. Unfortunately ZnSe is brittle and the grooves suffered from severe chipping. As a result the diffraction efficiency was low and there was a large amount of scatter.

Guay and his coworkers[15] in Canada describe the use of laser ablation at 532 nm to fabricate diffractive optical elements in ZnSe. Although the lowest diffracted orders were detected at 10.6 µm, the groove walls were very rough due to the redeposition of ablated material. Such a grating would not be useful for spectroscopy.

Kurisu et. al.[16] fabricated diffractive optical elements in ZnSe through the use of photolithography and reactive ion etching. They used a 16 step pattern (4 binary bits) to create arbitrary surface profiles. The primary application was beam splitting and beam shaping of a 10.6 µm laser. Much work would be required to perform acceptably at much shorter wavelengths or in spectroscopic applications.

As reported previously, the baseline for fabricating the WINERED grating was nanoprecision 3D grinding[12]. However it proved very difficult to maintain the sharp groove corners required for high diffraction efficiency due to wear at the edge of the grindstone. Work on LLNL on diamond flycutting high quality gratings in germanium indicated an alternative. Good results in test cutting grooves onto 1 inch diameter discs of ZnSe[10] set the stage for the cutting of a much larger ZnSe grating. The results of these experiments will be reported in the following sections.

3. CUTTING THE GRATING

In August 2008 all the hardware was in place to cut a grating on a large ZnSe prism. This would not be the final grating for WINERED but a somewhat smaller prism, identical in shape, to serve as a proof of concept. The prism supplied by II-VI had angles of 90, 70 and 20 degrees and a rectangular entrance face 23 x 50 mm in size. The grating area is approximately 50 x 58 mm. We specified a 5º tilt between the entrance face and the body of the prism to separate front

surface reflections from the diffracted beam. All surfaces of the prism were polished at the vendor. The flatness of the entrance face was 0.64 wave p-v and that of the prism hypotenuse, where the grating would be cut, was 0.85 wave p-v.

A mounting fixture was machined from tool steel to support the ZnSe prism on a translation stage of the PERL II ultraprecision lathe. The fixture has three support pads each with a central hole connected to a vacuum pump hold the prism in place. A small amount of vacuum grease around each pad provides a leak tight seal. Figure 1 is a photograph of the setup just before the start of machining. The machine resides in a temperature-controlled enclosure, which sits within a temperature-controlled room.

The machining procedure is very similar to that used to cut germanium gratings at LLNL. A diamond tool cut to match the desired groove shape rotates in the lathe spindle at 1000 rpm. The stage holding the blank translates horizontally and orthogonal to the axis of rotation to cut a groove. The speed of the translation for cutting ZnSe is 0.4 inch/minute as determined by previous experiments. At the end of each groove the spindle is incremented forward by the groove period. The translation stage then moves in the opposite direction to cut the next groove. This process repeats until the grating is complete. A laser interferometer controls the motion of both the stage and the spindle to ensure precise groove positioning and the absence of periodic error. A steady spray of light mineral oil is directed toward the point where the tool contacts the blank to provide for cooling, lubrication and the removal of chips.

Once the spindle is started the translation stages remain off for an 8 hour "soak" during which all mechanical components and the air within the enclosure come to thermal equilibrium. The actual cutting began at 4:15 PM on 8/5/08 and was completed at 4 PM on 8/12/08. At the end of the process the grating is removed from the machine and cleaned using isopropyl alcohol and a soft artist brush. Unlike previous experiences with germanium, many small particles of zinc selenide remain stuck to the surface of the grating after the brush cleaning. This is believed to be due to electrostatic attraction as ZnSe, unlike Ge, is a good insulator. An application of the peel off coating OptiClean following the manufacturer's directions was very effective in removing the residual particulates[17].

Once clean the first test of the grating is a microscope inspection, the results of which may be seen in figure 2. Under bright field illumination, the grooves appear quite clean and sharp with little evidence of chipping. The next test is to place the grating in front of a Zygo interferometer and examine the deviation from an ideal plane wave of the diffracted wavefront. One would prefer to perform this test in immersion but the return signal is too low due to the relatively low reflection of the ZnSe-air interface and also due to attenuation and scatter loss in the material. Instead the Zygo test is done with a direct reflection off the grating surface. Here is where a problem was discovered. The interferogram from the 70º blazed facets, as shown in figure 3, reveals large wavefront aberrations, too large to be accurately measured by the Zygo. An eyeball estimate of the wavefront error is 5 to 7 waves p-v, which is very poor. An interferogram from the 20º blazed facets registered a wavefront error of nearly 3 waves p-v and 0.56 waves rms. The interferometric test results are corroborated by the simple experiment of illuminating the grating with the beam from a red diode laser. The diffraction pattern appeared smeared, not the clean spots one would expect.

It was a big puzzle why a coarse grating cut on a one inch ZnSe disc in October 2007 had very good (0.30 wave p-v) wavefront error[10] and the large ZnSe grating cut 10 months later on the same machine had several waves of aberration. Experiments with a capacitive distance transducer mounted on the translation stage showed its position relative to the spindle drifted nearly 2 μm over 24 hours, greatly exceeding the design specification of the machine. Further experiments with temperature sensors showed the cause to be a complete loss of temperature control in the PERL room and enclosure. The root cause was traced to a water leak earlier that year on the floor above PERL that ruined the room temperature controller. Due to plans to consolidate facilities in another building, the finely tuned temperature control system was replaced by an industrial grade thermostat (as a temporary measure). The thermostat remained in place when the moving plans were later cancelled.

There are a number of things that we learned from this first attempt at cutting a large ZnSe grating. The degradation of the thermal control system was an unexpected surprise. It took over a month to restore the original system and to achieve previous levels of room temperature control. Some time was also spent retuning the enclosure temperature control system. Based on this experience we instituted the practice of running a several day test of machine drift prior to all future attempts to cut gratings. These drift checks included the use of a capacitance gauge and several temperature sensors located around the room, in the enclosure and on the spindle.

Despite the fact that this first attempt yielded an unusable grating there were some reasons for optimism. The grooves looked good under 100x optical inspection. The wavefront error was poor, but the cause was identified and fixed. With the restoration of thermal control there was reason to expect a reduction to levels seen in previous small gratings (e.g. 0.3 wave p-v).

4. FIRST RECUT

After several months of repairing, testing, and fine tuning the PERL temperature control system, we were ready for another try at cutting the grating. The large ZnSe prism was expensive (~$8K) and there was a 10-12 week lead time on the procurement. So we chose to recut the grating on the existing piece rather than purchase a new blank. We had had good success simply cutting a new grating over the old one working with germanium. The tool was set to cut about 10 μm beneath the existing grating.

The cutting started at 11:15 AM on 12/25/08 and was completed on 1/1/09. Between midnight and 2 AM on 12/30 the polyurethane tubing carrying mineral oil coolant to the spray nozzle sprung a pinhole leak. Oil sprayed the inside of the PERL enclosure. The bottom of the enclosure was essentially flooded. For a number of hours there was no oil flow to the workpiece or diamond tool. The coolant line was replaced within 8 hours and the cutting continued.

The grating was removed from the machine and cleaned as before. Visual inspection with an optical microscope showed an immediate problem. There was bad chipping of the grooves that did not seem to be related to the oil leak and the interruption of coolant (see figure 4). Chipping of a groove edge may indicate a weakness or flaw in the substrate material that breaks off with less force than required to cut a clean edge. It may also indicate that the cutting is occurring in brittle mode instead of a ductile mode.

A Veeco optical profilometer was used to measure surface roughness. The average value was 8.5 nm along a profile at a few degree angle to the groove direction. The true random roughness will be somewhat less because the component orthogonal to the groove contains a contribution from the tool shape (i.e. edge not perfectly straight).

We next placed the grating in the Zygo interferometer to measure the wavefront error in the diffracted beam. We were interested to see the improvement with properly functioning thermal control. The results can be seen in figure 5 and are quite good. The values of wavefront error in reflection from the 70º blazed facets are 0.77 wave p-v and 0.13 wave rms measured across the grating.

These values compare favorable with the design requirements given in section 2, which calls for ≤1.0 wave p-v error measured in immersion at 1.0 μm wavelength. The corresponding requirement in reflection, correcting for the 633 nm wavelength of the Zygo data and for the 2.49 refractive index of ZnSe at 1.0 μm, is ≤0.63 wave p-v. Our grating exceeds this by about 20%. However a better gauge of the wavefront error is the rms measurement, which averages over the entire surface. For random error 0.63 wave p-v is equivalent to 0.18 wave rms and our grating is clearly below this value.

Further information may be drawn from the Zygo measurements. If one views the 2-D representation of wavefront error it is clear that the error varies along different directions across the wavefront. Specifically, the error along a direction parallel to the grooves is much less than that across the grooves. That is because they represent different fabrication time scales. An individual groove is cut in 5 minutes. The error here demonstrates intrinsic short term stability which is the ultimate limit of the machine. For this case these values are 0.07 wave p-v or 0.02 wave rms (see figure 6). Error across the grooves (~0.5 wave p-v) represents environmental drift over 7 days and can potentially be reduced by tighter control.

Two things were learned from the second trial of cutting a large grating. Most importantly the thermal issues experienced on the first trial have been resolved and the wavefront error on the grating meets the design requirements. Unfortunately the grooves were badly chipped making this grating unusable. We believe that this was due to cutting a grating into a substrate that had residual subsurface damage produced by the first trial. For the next trial we would need to either procure another prism blank or remove the existing grating surface features by polishing. The polishing must be deep enough to remove any residual damage from the prior cutting and must not create any damage of its own.

5. SECOND RECUT

Due to the problem of chipping on the first recut we decided to remove the grating surface features by polishing. This we hoped would remove any subsurface damage introduced by the machining while avoiding the creation of more damage. The polishing with 3 μm diamond abrasive was performed on 6/17/09. When complete, the hypotenuse was flat to within four waves.

Programmatic work tied up the PERL for most of the year and limited its availability for the ZnSe grating work. We were not able to recut the grating until late in the year.

Based on excellent results in germanium[18], we changed our fixturing procedure to use cyanoacrylate adhesive to bond the ZnSe in place instead of relying on vacuum. This would also eliminate any susceptibility to variation in or loss of vacuum pressure. The diamond tool was inspected after some cutting experiments in zinc sulfide. Some signs of tool wear were seen and we had the tool refaced before starting the grating.

To verify temperature stability prior to beginning cutting the grating we ran a machine drift check. Peak to peak temperature variations were measured of 0.25ºC for the room, 0.025ºC for the machine enclosure and <0.01ºC for the machine spindle. These values indicate excellent environmental control. We reduced the feed rate slightly, from 0.40 to 0.35 inch per minute in an effort to reduce chipping.

The cutting started at 8 AM on 12/8/09 and was anticipated to last 7 days. However on the morning of 12/13 the PERL was discovered to have executed an emergency stop (e-stop) on the previous day. The cutting was about 70% complete when the machine halted. The immediate cause of the e-stop was that the z-stage, on which the spindle rides, was driven to its limit of travel. Further investigation determined that the z-stage was not moving (i.e. tool was in a groove) when a control error occurred that drove it to the limit of travel. This indicated that the problem was in the laser interferometer that determines position and not in the control system. We found traces of oil on the interferometer optics that attenuated the beam strength to point of causing errors. The oil had been apparently accumulating for a number of years through some open holes in the spindle frame (see figure 7). Once the optics were cleaned and the holes plugged, the laser interferometer performed normally.

We wanted to characterize the cutting, even though the grating was incomplete. So the grating was removed from the machine and cleaned as before. The ZnSe residue from the machining seemed especially heavy. It was dried and caked on over the grooves. Perhaps the oil flow had been lower than optimal. Once clean, a microscope inspection showed pitting on the flat regions of the groove faces (see figure 8). This is something that had not been seen in previous machining and seemed to get worse as the cutting progressed. The groove edges did not appear chipped.

We performed an interferometric measurement of the wavefront error of the grating in reflection and got 0.61 wave p-v and 0.11 wave rms. (See Zygo data from the 70º facets in figure 9.) These are acceptable values and are slightly better than those achieved on the first recut. This dataset was then masked down to a 7.5 mm diameter subaperture at several positions across the full aperture. Figure 10 shows the WINERED requirement for spectral resolution is met.

One of the lessons of the second recut is that we can consistently meet the wavefront error requirement when we have good temperature control. Also chipping can be eliminated or at least greatly reduced when the grooves are cut into a smooth polished surface. However the new pitting observed on the groove faces seems to indicate that the polished surface was not damage free.

A review of the literature shows that mechanical polishing can produce subsurface damage in ZnSe[19]. Diamond machining has also been demonstrated to cause damage[20]. There are known ways to remove material without damage. These include chemical etching and chemical mechanical polishing or CMP. We have used a HNO_3:HF:CH_3COOH etch to remove damaged surface layers in germanium[9]. Reference 18 mentions the use of HCl as an etchant for ZnSe. Care must be exercised as toxic H_2Se is released in the process.

CMP, which relies on an alkaline slurry of colloidal silica, has been used in the semiconductor industry to provide a damage-free polish on silicon wafers. However it has been shown to produce small but measureable damage in ZnSe[21].

6. CONCLUSIONS AND FUTURE WORK

We made 3 attempts to machine a ZnSe immersion grating as a subscale prototype for the WINERED spectrograph. The grating area was an order of magnitude larger than gratings previous cut on this machine. None of attempts was completely successful due to different mechanical failures. The failed components were all repaired or replaced. We have now implemented a checkout procedure to qualify the machine performance before a new grating cut is started.

With proper thermal control the requirement on the full aperture diffracted wavefront error has been met. The remaining problem is chipping and pitting of the grooves, which can lead to ghosts in the spectrum[10]. We believe that this effect is caused by subsurface damage in the grating substrate produced by polishing or prior diamond machining. A damage free substrate is required before machining and can be obtained by chemical etching. We plan to verify this hypothesis using one inch diameter discs of ZnSe. When high quality gratings can be consistently cut on the small discs, then we will re-cut the large grating. An important lesson learned was to not be anxious to scale up to large substrates. All process development should be done on small parts. They can be cut much more quickly providing rapid process feedback. They are also much cheaper and can be preserved for future examination and testing instead of being recut.

ACKNOWLEDGEMENTS

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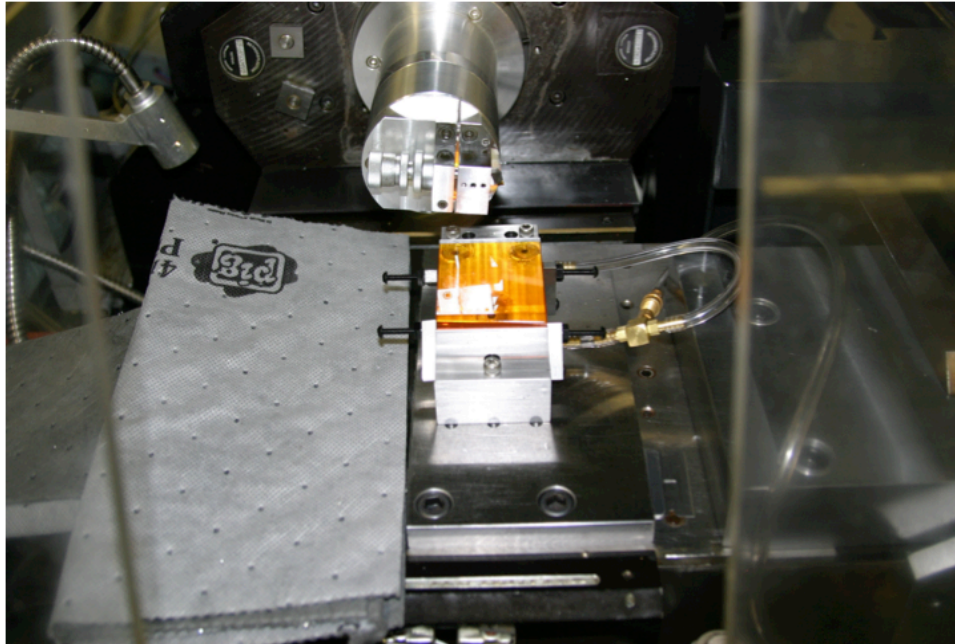
Figure 1. ZnSe grating blank held in vacuum chuck inside the PERL II ultra-precision lathe prior to the start of cut.

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Figure 2. Magnified image of grooves (period is 31.73 μm) from first cut of grating. Cutting done on on polished substrate as received from vendor.
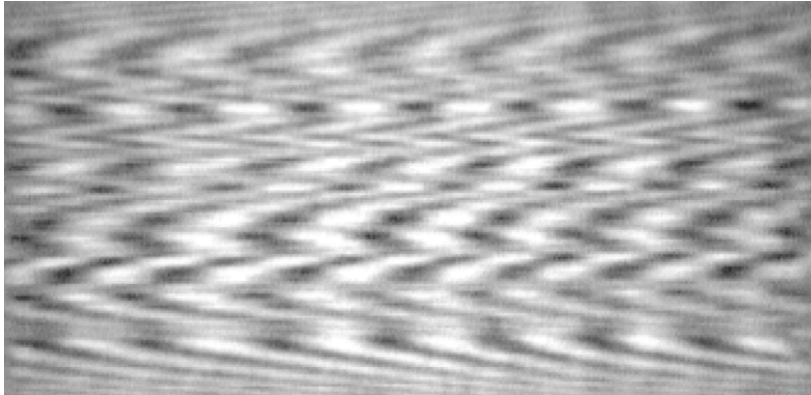
Figure 3. Interferogram of diffracted wavefront reflected from 70º blazed grooves. Inoperative thermal control during first cut of grating results in 5 to 7 waves p-v @633 nm of wavefront error.
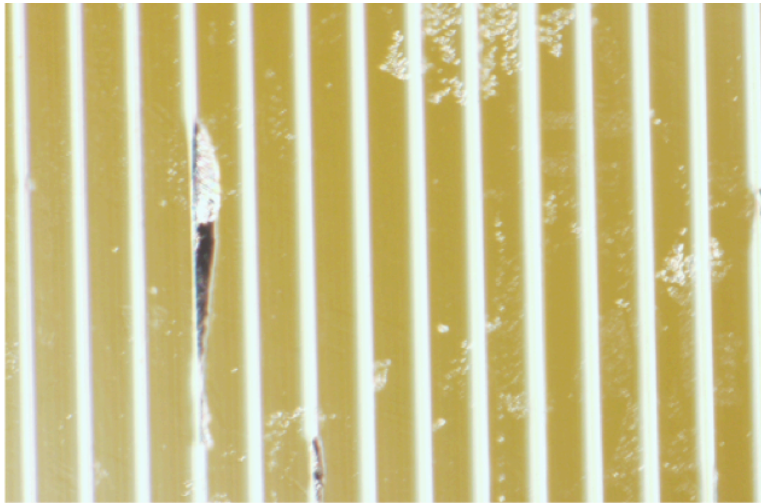

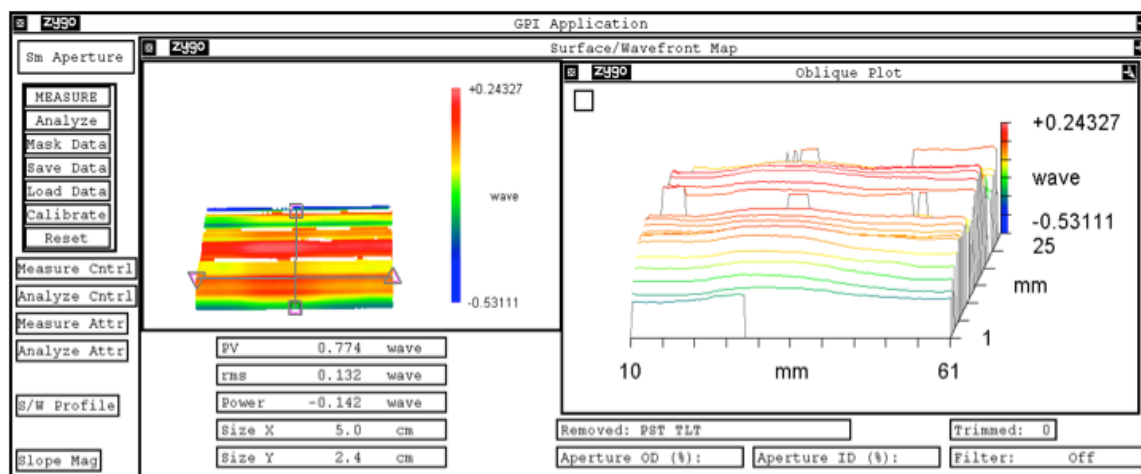Figure 4. Magnified image of grooves on first recut (grating cut over existing grating) shows bad chipping.

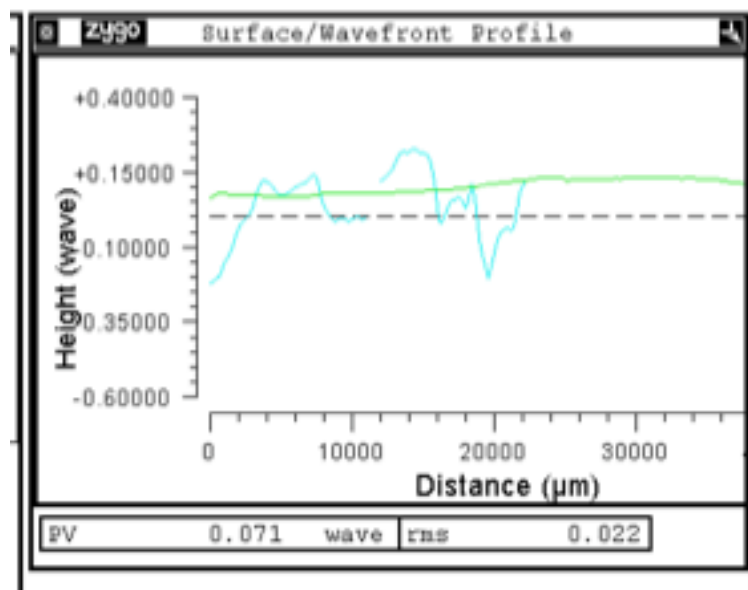Figure 5. Wavefront error from first recut shows much improvement with thermal control performing well.

Figure 6. Plot of surface profile along a groove (smooth line) and across all the grooves in the grating. Actual paths are shown in figure 5. Along a groove the wavefront error is small, 0.071 wave p-v and 0.022 wave rms
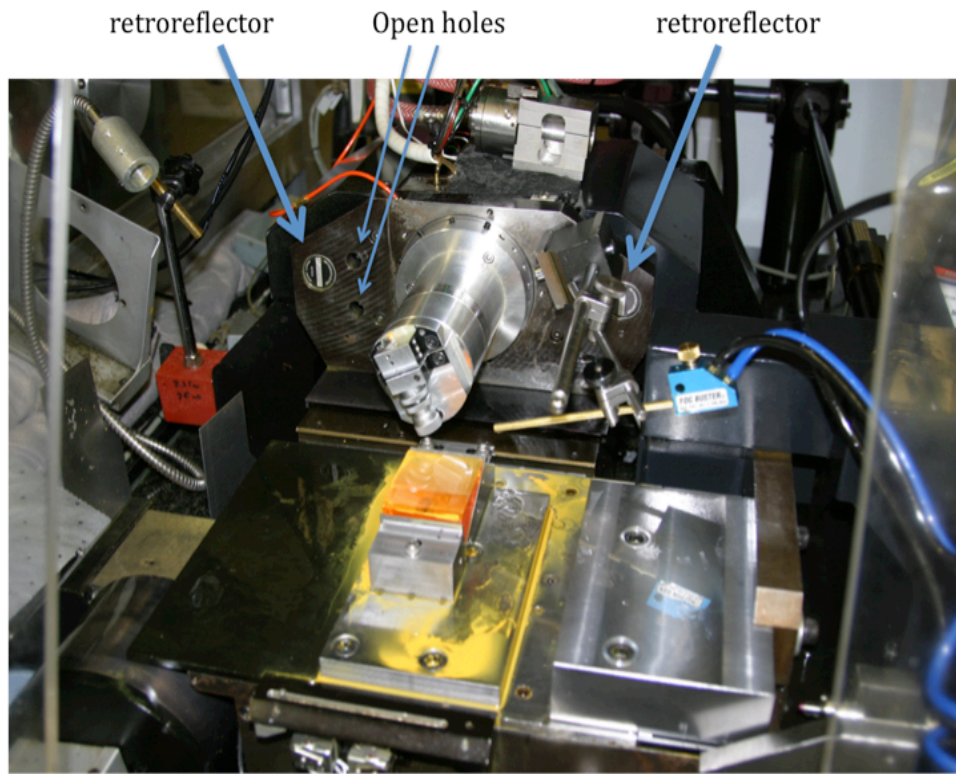
Figure 7. Machine configuration after the second recut shows partially cut grating is still in the holder. The retroreflector that had accumulated a coating of oil and the holes through which the oil may have entered are indicated.
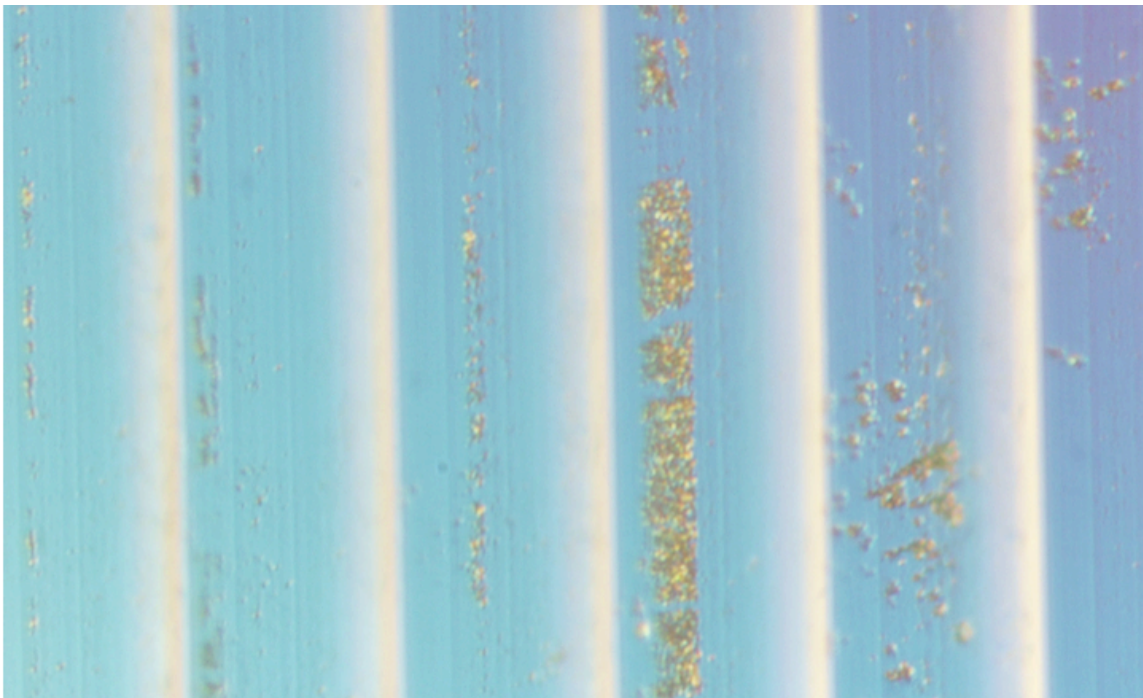

Figure 8. Magnified image of grooves produced on second recut shows no chipping but does show pitting of the groove faces.
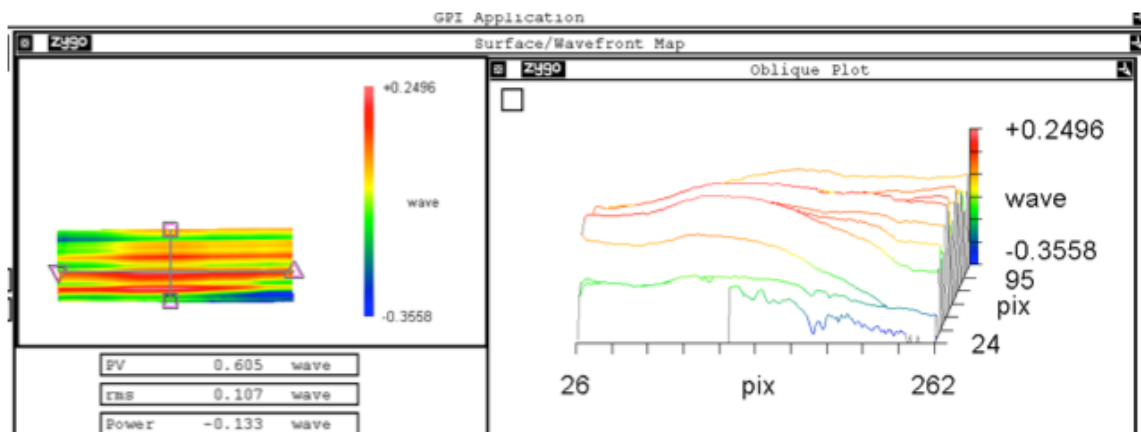
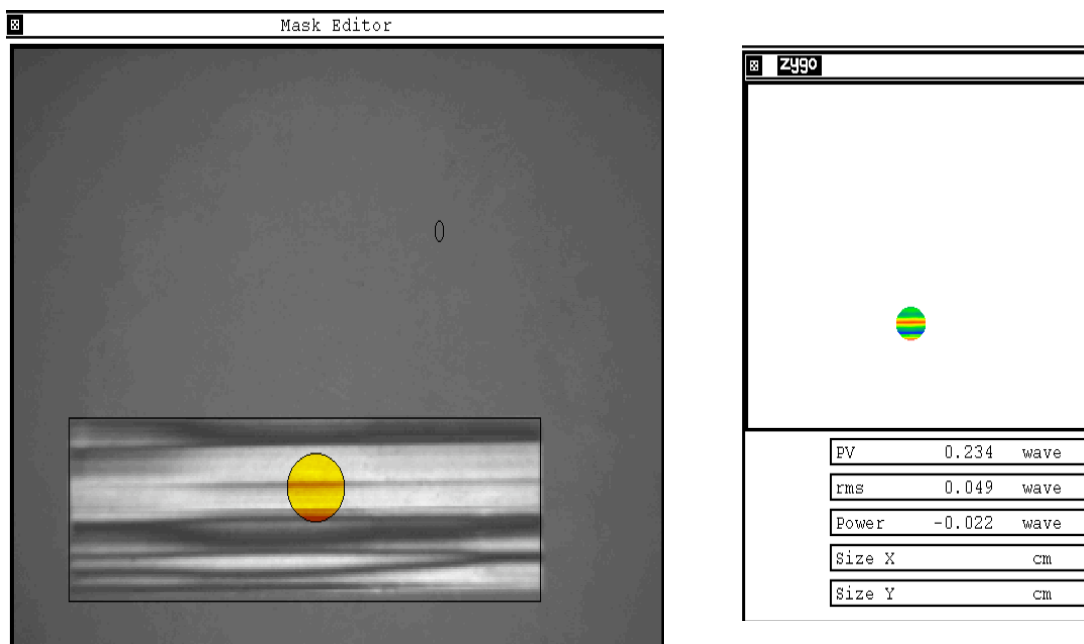Figure 9. Wavefront error from grating produced on second recut shows some improvement over first recut.

Figure 10. We set a subaperture mask of 7.5 mm diameter at four points across the full grating aperture. The values of rms wavefront error were 0.045, 0.049, 0.071 and 0.074 waves, all of which meet the WINERED requirement for spectral resolution. The data shown above is from the subaperture nearest to the center of the full aperture.